# Modeling of electronic properties of interfaces in solar cells

Annegret Glitzky and Alexander Mielke

Funding period 06/2010 - 05/2014
Requested funding: 1 position

DFG Research Center MATHEON
*Mathematics for key technologies*

WIAS
Weierstraß-Institut für Angewandte Analysis und Stochastik

January 19, 2010

# Aim / topic / background of project

In 2008, MATHEON has started activities in **PhotoVoltaics**

- MATHEON Industry Workshop 6.–9. October 2008

  ***Technologies of Thin-Film Solar Cells***

  Org.: A. Münch, B. Wagner, V. Mehrmann, B. Rech (HZB)
  Industry partners: Leybold Optics, Carl Zeiss AG, Schott AG, IBM.

- Participation in **PVcomB**

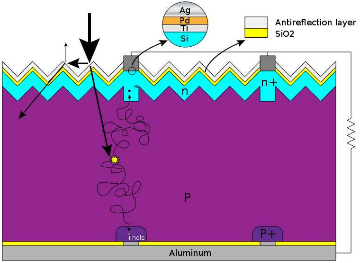
  ***Competence center for thin-film and nanotechnology for photovoltaics Berlin***

  - HZB, TUB, FHTW, MATHEON, IHP, U Potsdam, FZ Jülich
  - V. Mehrmann, A. Mielke, F. Schmidt, B. Wagner
  - Exp. budget: 18 M € for five years, including
  - 3 positions for Mathematical Methods in Photovoltaics

**Present proposal:**

Improve mathematical modeling in cooperation with HZB

# Aim / topic / background of project




## Technological aims in photovoltaics:

- maximize efficiency of the **solar cells**
- minimize production costs, ...

## Principle of solar cells:

- Photons generate electron-hole pairs
- electrons/holes move to contacts

$\rightsquigarrow$ minimize recombination losses

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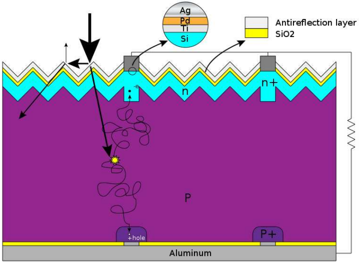


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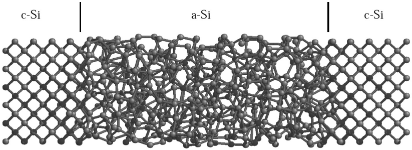
At heterointerfaces new electrical effects may occur:

- electrons, holes are transmitted/reflected
- technological treatment of interfaces leads to defect distributions
- special recombination at defects
- quantum mechanical tunneling effects

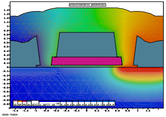



$\rightsquigarrow$ new mathematical models required!

# Contributions of the principal investigator

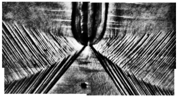
## RG 1 of WIAS:

Analytical treatment of semiconductor models
Numerical simulation of semiconductor devices
Multiscale modeling, homogenization, dimension reduction



## A. Mielke:

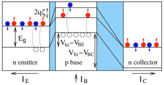
Multiscale modelling for evolutionary problems
Abstract existence results for geometric gradient flows
Γ convergence applied to evolutionary problems

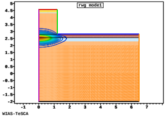


## A. Glitzky:

Analysis and numerical analysis for
- Spin-polarized drift-diffusion models
- Electro-reaction-diffusion systems

Energy models for semiconductor devices
WIAS-TeSCA simulations of semiconductor lasers



## (1) Modeling and analysis of nontrivial interface conditions

- **Equations in the bulk** for $n$, $p$, $\varphi$, $\eta =$ defect-occupation probability

$$\frac{\partial}{\partial t} n - \mathrm{div}\big(c_n(\nabla n - n\nabla\varphi)\big) = G_{\mathrm{phot}}(t,x) - \langle\!\langle \rho_n(..,n,\eta)\rangle\!\rangle - R(n,p),$$
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$$-\mathrm{div}\big(\varepsilon(x)\nabla\varphi\big) = d_{\mathrm{dop}}(x) + p - n - \langle\!\langle \eta\rangle\!\rangle \quad \text{where } \langle\!\langle g\rangle\!\rangle := \int_{E_{\mathrm{V}}}^{E_{\mathrm{C}}} g(E)N(x,E)\,\mathrm{d}E$$
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- **Interface conditions** at $x^{\mathrm{I}} = x = x^{\mathrm{II}}$

- extra defect dynamics ($\widehat{\eta}$ localized at interface $x$)

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- current determined by thermionic emission and defect recombination

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**Aims:**
- thermodynamic wellposedness of resulting model equations
- existence theory for stationary/time-harmonic/instationary problems (starting from lower dimensional problems)

## (2) Approximation by pseudo layers

For numerical implementations it is common practice to replace the interface conditions and the interface-trap kinetics by bulk kinetics on thin layer elements with suitably scaled properties.

(++) classical interface conditions can be used
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### Aims:

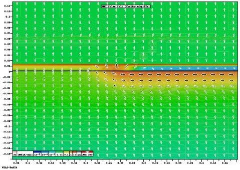
- Investigate this approximation procedure in a rigorous fashion,
- Which nontrivial boundary conditions can be obtained by such limits? How much freedom do we have in such approximations?
- Approximate tunneling effects through interfacial potential barriers:
  Do pseudo-layers with fitted material data approximate the tunneling characteristics sufficiently well?

## (3) Numerical approximation and simulation

1-dimensional software AFORS-HET of Helmholtz Zentrum Berlin (HZB) uses finite differences, no numerical analysis available

### Aims:

- establish discretization schemes benefitting from analytical properties of the continuous problem
- implement such schemes or adapt WIAS-TeSCA
- predict characteristics of solar cells (band diagrams, recomb. rates, carrier densities, electrostatic pot., cv-characteristics, quantum efficiency)
- validation of the models by comparison with measurements of HZB



WIAS-TeSCA Simulation (R. Nürnberg)
Electron current through a structured passivation layer in a thin film solar cell.

**Cooperations within Application Area D**
**D23** (F. Schmidt) "Design of nanophotonic devices and materials" (interplay of material properties of interfaces with their optical and electronic properties)

**Cooperations with other Application Areas of MATHEON**
**C10** (B. Wagner) "Modeling, asymptotic analysis and numerical simulation of interface dynamics on the nanoscale" (properties of surfaces, atomic layers)

**External Cooperations:**
Helmholtz Zentrum Berlin für Materialien und Energie, Group SE1 "Silizium-Photovoltaik", Prof. Bernd Rech, Dr. Rolf Stangl, Dr. Lars Korte (discussion of models, experimental data to validate our models)

MATHEON projects C10, D22, and D23 supply basic research for **PVcomB:** Photovoltaics Competence Center Berlin (Head Prof. Bernd Rech)